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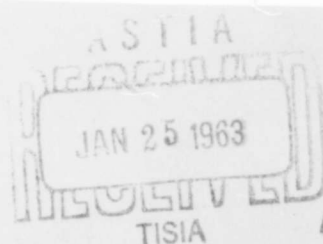
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CHEMICAL NON-EQUILIBRIUM EFFECTS
IN HYPERSONIC PURE AIR WAKES

M. LENARD
M. E. LONG
K. S. WAN



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SPACE SCIENCES LABORATORY

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MISSILE AND SPACE DIVISION

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SPACE SCIENCES LABORATORY

AEROPHYSICS SECTION

CHEMICAL NON-EQUILIBRIUM EFFECTS
IN HYPERSONIC PURE AIR WAKES*

by

M. Lenard, M. E. Long, and K. S. Wan

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ABSTRACT

1. The effect of finite chemical reaction rates on the chemical structure of hypersonic wakes is examined. The technique of incipient non-equilibrium coefficients, based on linearized chemical kinetics for a ~~seven~~⁷⁻ component (O_2 , N_2 , O , N , NO , NO^+ , e^-) ~~ten~~¹⁰⁻ reaction model of high temperature air, is utilized in the analysis.

2. The far wake is treated as an asymptotic region; the near wake theory considers the viscous mixing of the boundary layer flow with the inviscid and re-circulating flows in the base region, and the subsequent development of this viscous core into the wake region downstream. A range of altitudes and flight speeds of practical interest is considered. 3. The results show where non-equilibrium effects are important in the wake and whether they arise primarily from convective or diffusive effects. The species that are the principal contributors to the non-equilibrium effects are also identified.

The incipient non-equilibrium results are then related to calculations assuming chemically frozen flow. 4. By the application of chemical kinetics to the frozen results, it can be shown that the appearance of incipient non-equilibrium effects bears an inverse relationship to the validity of the frozen flow assumption for equivalent wake calculations.

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INTRODUCTION

Aerodynamics at hypersonic speeds is greatly complicated by chemical changes occurring in high temperature air. These chemical changes have significant effects on the thermodynamic and transport properties of air; in some cases, they give rise to diffusive phenomena which can contribute to the transfer of energy through the moving and chemically reacting fluid. In addition, the theoretical prediction of the chemical state of air in the wake is an important task for its own sake, because it determines the electrical transmission and radiative properties of the wake, which are important means for the detection, observation, and identification of hypersonic re-entry bodies.

For these reasons a great deal of current theoretical aerodynamic research has been directed towards predicting the chemical state of reacting air flows. Under many circumstances of practical interest in the re-entry problem, chemical changes will take place at rates which are comparable to rates at which changes occur in the flow due to fluid mechanic phenomena. Under these circumstances theoretical predictions must be based on simultaneous consideration of chemical kinetics and fluid mechanics. This is a very formidable problem, particularly in diffusive flows and for a chemical kinetic model that attempts to account for all the ionizing species in a physically meaningful way. For these reasons much of current research has been directed towards justifying simplifications that make the general problem of coupled chemical kinetics and fluid mechanics more tractable in specific situations.

The present investigation is directed toward solving this general problem for the specific case of uncontaminated air wakes behind bodies moving at hypersonic speeds. This type of flow is characterized by the presence of both convective and diffusive effects, but the latter (as in boundary layers) occur only along constant pressure surfaces. An approximation procedure, which is based on expanding the coupled fluid mechanic and chemical kinetic equations in powers of a small aerothermochemical parameter, is used to

describe these types of flow. The first term in the expansion describes the hypersonic wake corresponding to instantaneous local chemical equilibrium. The next term in the expansion, which is calculated in detail for several practically significant wake flows, indicates the deviation of the flow from the chemical equilibrium model due to the finite rate chemical kinetics. These deviations are due both to the rapidity of convection of the fluid particles along the wake streamlines and the inter-diffusion of the reacting species across the streamlines. The results show which of these non-equilibrium effects dominates in various parts of the wake and also which of the species are the major source of these effects. The analysis is based on a seven component (O_2 , N_2 , O , N , NO , NO^+ , e^-) ten reaction model of high temperature air.

METHOD OF ANALYSIS

The key equation that couples the chemical kinetics and the fluid mechanics in reacting flow problems is the equation of conservation for the chemical species that comprise the reacting mixture. For a mixture comprised of $n + m$ species with m independent conservation laws relating the species concentrations to each other (e. g. over-all mass conservation, charge conservation in a neutral plasma, etc.) there will be n independent species conservation laws of the following type;

$$\frac{DC_i}{Dt} + \frac{1}{\rho} \operatorname{div} \rho C_i \vec{q}_i = \frac{w_i}{\rho} (p, T, C_j, \dots) \quad (1)$$

In addition to equations (1) the usual fluid mechanic conservation laws for mass, momentum, and energy, the equation of state and other auxiliary equations relating thermodynamic and transport properties, are necessary to complete formulation of the general problem. However, due to the appearance of the chemical kinetic mass generation rate terms on the right hand side of equations (1) these equations are of particular significance in the following analysis.

In reference 1 it was pointed out that for "fast" chemical reactions it is possible to treat the general problem in terms of an expansion procedure. The expansion parameter for the procedure is the ratio of an appropriate chemical time, t_c (which is based on the sensitivity of the chemical mass generation rate functions to changes in composition) and a fluid mechanic reference time t_f . As a result of the expansion procedure incipient non-equilibrium coefficients can be defined for a reacting mixture, which can be used to predict non-equilibrium effects both qualitatively and quantitatively from properties of the flow solution based on instantaneous local chemical equilibrium. The latter type solutions are comparatively simple to obtain for wakes and other hypersonic aerodynamic problems of current interest. In what follows the results of reference 1 will be utilized in conjunction with equilibrium wake solutions; for proper interpretation of the results it is appropriate now to reiterate the salient features of the expansion procedure including the concept of incipient non-equilibrium coefficients as they apply to wake type flows.

If equations (1) are written in non-dimensional form the expansion parameter

$$\mathcal{E} = \frac{t_c}{t_f} \quad (2)$$

will appear explicitly in the equations as follows;

$$\mathcal{E} \left\{ \frac{DC_i}{Dt} + \frac{1}{Re Sc} \frac{1}{\rho} \operatorname{div} (\rho C_i \vec{q}_i) \right\} = \frac{w_i}{\rho} (p, T, C_j) \quad (3)$$

If now all dependent variables are expanded in powers of \mathcal{E} and terms grouped according to powers of \mathcal{E} in all the pertinent equations, the over-all conservation equations for the leading terms are unchanged (since the parameter \mathcal{E} does not appear in these equations explicitly), but species conservation equations (3) become for the leading term

$$\frac{w_i}{\rho} (p_1, T_1, C_{j1}) = 0 \quad (4)$$

where subscript 1 denotes the leading terms in the \mathcal{C} expansion. Equations (4) form an algebraic system which can be solved for the first order composition

$$C_{j1} = C_{jeq}(p_1, T_1) \quad (5)$$

without reference to any fluid mechanic problem, thereby decoupling the chemical problem from the fluid mechanics. This justifies use of the chemical equilibrium composition for these types of problems. The effect of the flow process on composition can be ascertained by considering the next term in the expansion of equations (3). Specializing now to axisymmetric steady wakes the next set of equations in the expansion of (3) become;

$$\begin{aligned} u_1 \frac{\partial C_{i1}}{\partial x} + v_1 \frac{\partial C_{i1}}{\partial y} - \frac{1}{y\rho_1} \frac{\partial}{\partial y} \frac{\mu_1 y}{Sc} \frac{\partial C_{i1}}{\partial y} = \\ = \sum_{j=1}^n \left. \frac{\partial w_i / \rho}{\partial C_j} \right|_1 C_{j2} + \left. \frac{\partial w_i / \rho}{\partial p} \right|_1 p_2 + \left. \frac{\partial w_i / \rho}{\partial T} \right|_1 T_2 \end{aligned} \quad (6)$$

This is a system of n linear algebraic equations for the unknown second order terms; formulation of the second order problem should be completed by considering corresponding expansions of the remaining conservation equations. However, using (5) in the left hand side, and (4) in the right hand side of (6) these equations can be written in a more immediately useful form:

$$\left. \frac{\partial C_{ieq}}{\partial p} \right|_T \dot{p}_c + \left. \frac{\partial C_{ieq}}{\partial T} \right|_p \dot{T}_{CD} + \left. \frac{\partial^2 C_{ieq}}{\partial T^2} \right|_p \dot{T}_D = \sum_{j=1}^n \left. \frac{\partial w_i / \rho}{\partial C_j} \right|_1 \Delta C_{j2} \quad (7)$$

where the quantities

$$\Delta C_{j2} \equiv C_{j2} - \left. \frac{\partial C_{jeq}}{\partial T} \right|_1 p_2 - \left. \frac{\partial C_{jeq}}{\partial T} \right|_1 T_2 \quad (8)$$

group all second order terms into one "composition deviation" term, and the terms

$$\begin{aligned}\dot{p}_C &\equiv u_1 \frac{dp_1}{dx} \\ \dot{T}_{CD} &\equiv u_1 \frac{\partial T_1}{\partial x} + v_1 \frac{\partial T_1}{\partial y} - \frac{1}{y \rho_1} \frac{\partial}{\partial y} \frac{\mu_1 y}{Sc} \frac{\partial T_1}{\partial y} \\ \dot{T}_D &\equiv - \frac{\mu_1}{Sc \rho_1} \left(\frac{\partial T_1}{\partial y} \right)^2\end{aligned}\tag{9}$$

account for the flow effects based on the first order (i. e. chemical equilibrium) solution of the wake. The linear algebraic system (7) is solvable for the ΔC_{j2} , furthermore, as pointed out in an earlier note⁽²⁾, the quantities

$$\frac{\Delta C_{j2}}{\dot{p}_C}, \quad \frac{\Delta C_{j2}}{\dot{T}_{CD}}, \quad \frac{\Delta C_{j2}}{\dot{T}_D}\tag{10}$$

can be calculated once and for all without considering any particular flow problem. Associating each of the species with the appropriate amount of chemical energy, which is required to create it from a low temperature reference state, incipient non-equilibrium coefficients can be defined which account for the combined effect of all the species:

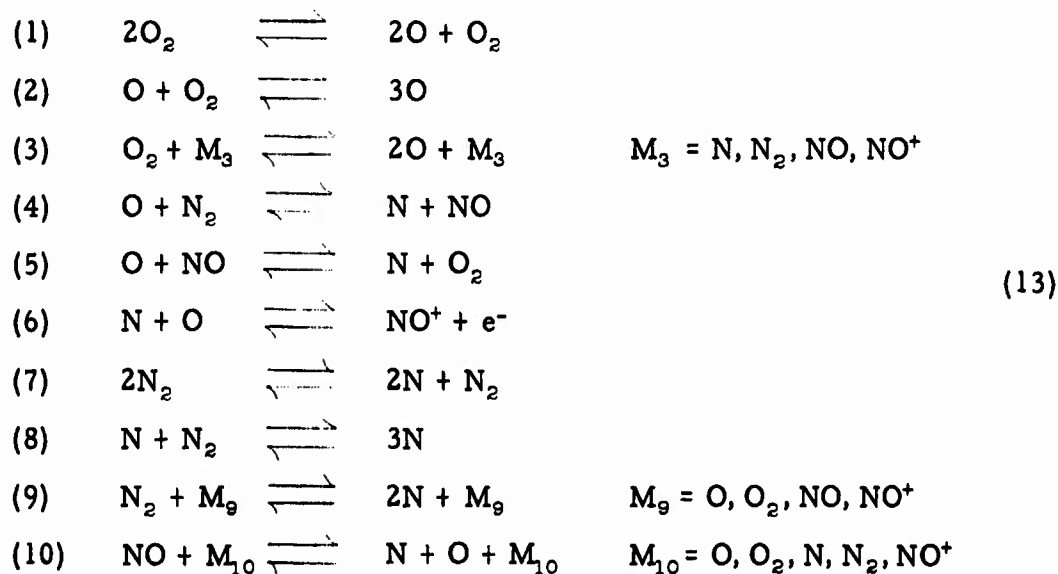
$$\begin{aligned}\frac{\Delta E}{\dot{p}_C} &= \sum_{i=1}^{n+m} E_i \frac{\Delta C_{i2}}{\dot{p}_C} \\ \frac{\Delta E}{\dot{T}_{CD}} &= \sum_{i=1}^{n+m} E_i \frac{\Delta C_{i2}}{\dot{T}_{CD}} \\ \frac{\Delta E}{\dot{T}_D} &= \sum_{i=1}^{n+m} E_i \frac{\Delta C_{i2}}{\dot{T}_D}\end{aligned}\tag{11}$$

For a given equilibrium wake solution the local value of enthalpy is known and the quantities in (9) can be calculated, so that the ratio

$$\frac{\Delta E}{h} = \frac{1}{h_1} \left\{ \frac{\Delta E}{\dot{P}_C} \dot{P}_C + \frac{\Delta E}{\dot{T}_{CD}} \dot{T}_{CD} + \frac{\Delta E}{\dot{T}_D} \dot{T}_D \right\} \quad (12)$$

can be calculated everywhere in the flow. This ratio, $\Delta E/h$, can be considered an indicator of incipient non-equilibrium effects in the flow. If it is small compared to 1.0 the equilibrium solution is valid. If the ratio is of the order or larger than 1.0 non-equilibrium effects are present in the flow. Due to the linearity of all the pertinent equations the causes of deviation from equilibrium can be ascertained both as to the fluid mechanic effect (i. e. convection, diffusion, etc.), from the magnitude of the various terms in (9); and as to the chemical species that are the principal cause on the deviation from equilibrium, from the magnitude of the various terms in (11).

Incipient non-equilibrium coefficients (11) have been calculated for a seven component (O_2 , N_2 , O , N , NO , NO^+ , e^-) ten reaction model of high temperature air given by Bortner and Golden⁽³⁾. The ten reactions that were considered are reiterated below for the sake of reference:



The results of these calculations, which are described in more detail in reference 1, were applied to two different types of wake calculations.

WAKE ANALYSES

A simple yet informative description of the far wake can be obtained by an analysis based on the asymptotic behavior of the disturbed fluid far from the body. The basic equation for this analysis is the momentum conservation integral:

$$C_D A = 4\pi \int_0^R \frac{\rho}{\rho_\infty} \frac{u_D}{u_\infty} y dy \quad (14)$$

where u_D is the velocity defect with respect to the free stream velocity:

$$u_D = u_\infty - u \quad (15)$$

and y is the radial distance from the centerline. The velocity and enthalpy are related by means of the adiabatic energy relation:

$$h + \frac{u^2}{2} = H_\infty \quad (16)$$

The total enthalpy of the flow H_∞ and the free stream pressure are both assumed to be constants. A compressibility transformation and Prandtl's mixing length analysis are then applied so that the description of the far wake is defined by:

$$\frac{u_D}{u_\infty} = \left(\frac{u_D}{u_\infty} \right)_{\max} [1 - \eta^{3/2}]^2 \quad (17)$$

$$\left(\frac{u_D}{u_\infty} \right)_{\max} = 1.72 \left[\frac{C_D A}{x^2} \right]^{1/3}$$

where η is the transformed radial coordinate;

$$\eta dy = \frac{\rho}{\rho_\infty} \frac{y dy}{R^2} \quad (18)$$

Equations (17) and (14) determine the variation of R with x:

$$\frac{R}{\sqrt{C_D A}} = 0.6 \left(\frac{x}{\sqrt{C_D A}} \right)^{1/3} \quad (19)$$

The details of the analysis are set forth in reference 4. Due to the lack of pressure gradient the quantity \dot{p}_C will be zero; the other two quantities in (17) can be calculated from the above analysis. (The turbulent Schmidt number is assumed to be one; this is consistent with the remaining assumptions.)

In the near wake analysis, the integral forms of the continuity, momentum and energy equations have been used. They are, when the external inviscid velocity and enthalpy gradients are neglected (reference 5).

Continuity Equation:

$$\frac{d}{dx} [\rho_e u_e \delta^2 \Delta] = \rho_e u_e \delta \left[\frac{d\delta}{dx} - \frac{v_e}{u_e} \right] \quad (20)$$

Momentum Equation:

$$\frac{d}{dx} [\rho_e u_e^2 \Theta \delta^2] = \rho_e u_e^2 \delta \left[\frac{d\delta}{dx} - \frac{v_e}{u_e} \right] - \frac{\delta^2}{4} \frac{dp}{dx} \quad (21)$$

Energy Equation:

$$\begin{aligned} \frac{d}{dx} [\rho_e u_e h_e \delta^2 \Theta_h] &= \rho_e u_e h_e \delta \left[\frac{d\delta}{dx} - \frac{v_e}{u_e} \right] \\ &+ u_e \delta^2 M \Theta_h \frac{dp}{dx} + \frac{2M\mu_e u_e^2}{Re_o} \Phi \end{aligned} \quad (22)$$

where

$$\Delta = \int_0^1 \frac{\rho u}{\rho_e u_e} \eta d\eta$$

$$\Theta = \int_0^1 \frac{\rho u}{\rho_e u_e} \frac{u}{u_e} \eta d\eta$$

$$\Theta_h = \int_0^1 \frac{\rho u}{\rho_e u_e} \frac{h}{h_e} \eta d\eta$$

$$\Phi = \int_0^1 \frac{u}{u_e} \left(\frac{\partial u / u_e}{\partial \eta} \right)^2 \eta d\eta \quad (23)$$

$$\eta = \frac{y}{\delta}$$

$$Re_o = \frac{\rho_o u_o \delta_o}{\mu_o}$$

$$M = \frac{u_o^2}{2h_o}$$

and δ is the viscous wake radius.

In addition, momentum and energy balances along the axis gave two more equations as:

$$\left[\rho u \frac{\partial u}{\partial x} \right]_{\eta=0} = -\frac{1}{2} \frac{dp}{dx} + \left[\frac{2\mu}{Re_o} \frac{\partial^2 u}{\partial y^2} \right]_{\eta=0} \quad (24)$$

$$\left[\rho u \frac{\partial h}{\partial x} \right]_{\eta=0} = \left[Mu \frac{dp}{dx} + \frac{2u}{Re_o Pr} \frac{\partial^2 h}{\partial y^2} \right]_{\eta=0} \quad (24)$$

Non-similar profiles for ρu and h were then assumed, i. e. ,

$$\frac{\rho u}{\rho_e u_e} = F(x_1 \eta) + a_1(x)(1-\eta^2) + a_2(x)(1-\eta^2)^2 + a_3(x)(1-\eta^2)^3 \quad (25)$$

$$\frac{h}{h_e} = G(x_1 \eta) + b_1(x)(1-\eta^2) + b_2(x)(1-\eta^2)^2 + b_3(x)(1-\eta^2)^3$$

Equations (20) to (25) are the basis of the near wake analysis. To start the near wake calculations, initial conditions near the "neck" must be known. In the present work, these conditions were obtained by using the analysis for base flow given in Reference 5. In that base flow analysis, the initial finite boundary layer at the corner of the base and its subsequent mixing with the inviscid and recirculating flows in the base region have been included in the treatment. Other factors affecting the solution are the Reynolds number, base wall enthalpy, base pressure values, and the inviscid flow conditions that were assumed. Therefore, these results give a more detailed and realistic description of the wake structure in the vicinity of/and further downstream of the "neck" region than can be obtained by means of the simplified treatment outlined above for the far wake. For particular near wake solutions the quantities in (9) were then calculated in order to assess incipient non-equilibrium effects.

DISCUSSION OF METHOD

It is quite evident that the expansion procedure that forms the basis of the incipient non-equilibrium analysis is not valid unless succeeding terms in the expansion are small throughout the flow field. This implies that if deviations from chemical equilibrium occurred in the flow field surrounding the re-entry body, application of this method to the wake could not be justified rigorously. However, the sensitivity of the chemical rate effects

to pressure and temperature seems to indicate that upstream effects play a minor role compared to local properties of the flow in bringing about non-equilibrium effects. This will tend to justify the use of incipient non-equilibrium coefficients on a local basis; it might also permit identification of chemically frozen flow regions where the values of the incipient non-equilibrium indicators $\Delta E/h$ are large.

In order to ascertain whether this is indeed so chemically frozen wake flow was assumed for the same flight conditions. The validity of this assumption was then tested by using the frozen composition and an appropriate local temperature to calculate the chemical mass generation rate terms for all the species. These terms were then compared to the diffusive terms in the species conservation equation on the basis of the chemical energy involved in all the species. The calculations utilize the fact that in the absence of pressure gradient and for a Schmidt number of 1.0 the relation

$$C_{i_{Fr}} = C_{i_{ref}} + \frac{u}{u_{\infty}} (C_{i_{\infty}} - C_{i_{ref}}) \quad (26)$$

identically satisfies the frozen species conservation differential equation provided u_{∞} , $C_{i_{\infty}}$, and $C_{i_{ref}}$ are all constants, independent of x and y . Then an "energy generation rate", due to the reactions

$$\dot{E}_R = \sum_{i=1}^{n+m} E_i \frac{w_i}{\rho} (p, T, C_{j_{Fr}}) \quad (27)$$

was compared to an "energy accumulation rate"; due to diffusion;

$$\dot{E}_D = \sum_{i=1}^{n+m} E_i \frac{1}{\rho y} \frac{\partial}{\partial y} \mu y \frac{\partial C_{i_{Fr}}}{\partial y} \quad (28)$$

If the ratio \dot{E}_R/\dot{E}_D is small frozen flow is justifiable. The outcome of this comparison depends greatly on the temperature chosen to calculate

the rates in (27) and on the reference condition that is used to calculate the frozen compositions in (26). For the far wake, the most "sudden" freezing would occur if the wake composition froze at a rear stagnation point behind the base. If the $C_{i_{ref}}$ are taken as the equilibrium composition corresponding to ambient pressure and the free stream stagnation enthalpy, the frozen wake composition profiles would exhibit the maximum possible deviation from the equilibrium assumption. Two temperatures were then used to calculate the reaction rates; the temperature corresponding to the equilibrium far wake solution is the lowest possible temperature, the actual temperature might be higher, the maximum being a temperature corresponding to the completely frozen composition described by equation (26). Neglecting any effect of composition on the equation of state, the enthalpy profiles in the far wake were assumed to be unchanged from equations (16) and (17), so that a "frozen temperature" could be calculated by:

$$h = \sum_{i=1}^{n+m} C_{i_{Fr}} h_i(T_{Fr}) \quad (29)$$

where the species enthalpies are given functions of temperature.

Steps (26) through (29) were performed for the near wake also. The free stream condition in (26) was replaced by the external (inviscid) condition used in the near wake analysis, and the appropriate reference conditions needed in (26) was taken as the surface condition at the trailing edge of the body. (This corresponds to a catalytic wall assumption.) The remaining assumptions of unchanged enthalpy and velocity profiles (as compared to the equilibrium solution) were made again. The presence of a pressure gradient in the near wake (which invalidates result (26)) was minimized by an appropriate choice of external conditions.

NUMERICAL RESULTS

Numerical calculations were performed for the far and near wakes for the flight conditions listed in Table I. For the equilibrium far wake, velocities, temperatures, enthalpies, and chemical energies along the centerline are given in Figures 1 through 3, respectively. The chemical energy (E_{chem}) is the energy absorbed by dissociation and ionization; when compared to h it is an indicator of the potential significance of chemical effects. Figure 4 shows $\Delta E/h$, the incipient non-equilibrium index (I.N.I.), for the same six cases along the far wake centerline. Since the temperatures are the highest near the centerline, for a 1 foot body ($\sqrt{C_D A} = 1.0$) this figure indicates the existence of an equilibrium region with the far wake (where the I.N.I. is less than 1.0) at only 3 of the 6 conditions studied. Near the body N is the largest contributing species to the I.N.I., whereas further downstream it is O. It is noteworthy that as the temperature drops, the I.N.I. first takes a downward turn for many of the cases and then begins to rise. This phenomenon is due to the fact that in spite of the lower rates at the lower temperatures, the tendency to deviate from equilibrium becomes smaller because of the diminished supply of N atoms that are "required" to recombine, and the simultaneous "flattening" of the wake profile which implies a decrease in the rates that are "prescribed" by the equilibrium wake solution (i.e., the terms in equation (9) become smaller). However, as soon as O recombination begins to take place, the tendency to deviate from equilibrium becomes several orders of magnitude larger. One may, for example, surmise from these results that for the high altitude condition (case 1), both the N and O recombinations will lag far behind, whereas at lower altitudes (e.g., cases 3 and 4) most of the N atoms will have recombined along the centerline; the excess atoms in the far wake will be mostly O atoms. This might have important consequences regarding electron

densities, due to the increased occurrence of NO^+ ions in regions where both type of atoms are present.

Figures 5 through 7 show properties of a particular equilibrium far wake profile as to velocity, temperature, enthalpy, chemical energy and composition. A station $383 \sqrt{C_C A}$ downstream from the body for case 3 was chosen as the example. Figure 9 shows the corresponding I. N. I. profile, showing also the separate effects of convective and diffusive terms. It is clear that, except at the wake center, interdiffusion of the reacting species is the dominant reason for deviating from chemical equilibrium in the far wake. This interdiffusion is due both to the curvature of the temperature profile $\left(\frac{\partial^2 T}{\partial y^2}\right)$, and to the curvature of the equilibrium composition vs. temperature variation in conjunction with the temperature gradients $\left(\frac{\partial T}{\partial y}\right)$, as shown in Figure 10. (Curvatures of the equilibrium composition profiles (Figure 7) also indicate the regions where there will be no diffusion.) The breakdown of the convective effect into axial and radial components (Figure 11) further demonstrates the utility of the method. Figure 12 indicates contribution of the various species to the I. N. I., atomic N and O dominate near the center and in the outer region of the far wake, respectively; the contribution of NO appears to be significant only at a narrow intermediate region.

Figure 8 compares I. N. I. profiles in the far wake for three different cases. Comparison of cases 3 and 4 shows the effect of altitude; whereas comparing cases 4 and 5 the effect of flight speed at the same altitude can be ascertained. As expected, low altitudes and high speeds (and the ensuing high temperatures) will extend the regions of equilibrium flow both laterally and axially. This is even more clearly shown on Figure 13 where the contours of $\Delta E/h = 1.0$ are plotted on a wake map for the three cases where equilibrium regions did occur. The effect of body size on these contours for one of the cases is also shown, indicating that the equilibrium flow regions will be different for various size and shape re-entry bodies.

Similar calculations were performed for several near wake profiles. Temperatures, enthalpies and chemical energies are shown in Figures 14 and 15, respectively. The I. N. I. profiles are shown in Figure 16. They show that for the high altitude condition (cases 7 and 8) the equilibrium assumption is not at all reasonable. It is less reasonable than in the corresponding far wake (case 2), in spite of the considerably higher temperatures and somewhat higher pressure near the base. The reason for this is partly the more rapid variation of fluid properties due to the large gradients near the base (i. e., \dot{T}_{CD} and \dot{T}_D are large) but mainly the fact that at this pressure there is a great deal of variation in the $N_2 - N$ equilibrium at the higher temperatures, whereas (as mentioned previously) at the lower temperatures only small chemical change is "required" by the equilibrium solution until the temperature is sufficiently low for the O recombination reaction to begin. At the lower altitude, the equilibrium assumption appears justified in some regions of the near wake at high wall temperatures (case 10). For case 9, Figure 17 indicates the separate effects of diffusion and convection on the I. N. I.; in contrast to the far wake, convective effects dominate in the near wake.

To augment calculations of incipient non-equilibrium effects, completely frozen wake flow was assumed for equivalent cases, and the validity of this assumption was then tested (equations 26 through 29). The results for the far wake are shown in Figures 18 through 24. Frozen temperature variation for the six cases along the centerline is given in Figure 18. Figures 19 and 20 show the variation of the ratio \dot{E}_R/\dot{E}_D along the centerline for the assumptions of equilibrium and frozen temperature, respectively. If this rate ratio is less than 1 frozen flow is justifiable. These results show that, considering the maximum possible temperature, frozen flow does appear justifiable for case 1 only. Figure 21 shows the frozen temperature profile $383\sqrt{C_D A}$ downstream for case 3; Figure 22 shows the rates \dot{E}_R and \dot{E}_D and their ratios for the equilibrium and frozen temperature assumptions, respec-

tively. These results, as the previous one, indicate the presence of a large "intermediate" flow region in the wake. Figures 23 and 24 indicate the effect of the various species on the rates for the same profile, the effects of O and N appear to dominate in various regions of the wake.

Finally, Figures 25 through 27 show similar calculations for the four near wake cases. Frozen temperatures, and the rate ratios for the equilibrium and frozen temperature assumptions respectively are shown in these three figures.

SUMMARY

Incipient non-equilibrium coefficients were found to be a practical and versatile research tool in estimating the effects of finite rate chemical kinetics in complicated hypersonic wake flow models. It was possible to account for both convective and diffusive effects in a multicomponent reacting mixture. The incipient non-equilibrium coefficients and the application of chemical kinetics to chemically-frozen wake calculations can be used to bracket the need for calculations accounting for coupled fluid mechanic and chemical kinetic effects in wakes. The results indicate that the concept of "sudden freezing" may be useful in flow regions near the body, where large gradients occur; but further downstream a large intermediate region appears where neither chemical equilibrium or chemical "freezing" can be justified.

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NOMENCLATURE

A	reference area for far wake drag
C_i, C_j	mass fraction of $i^{\text{th}}, j^{\text{th}}$ species
ΔC_{i2}	composition deviation (equation 8) for i^{th} species
C_D	drag coefficient
$\frac{D}{Dt}$	convective derivative
E_{chem}	chemical energy in mixture $E_{\text{chem}} = \sum_{i=1}^{n+m} E_i C_i$
E_i	chemical energy for i^{th} species
ΔE	energy deviation (equation 11 and 12)
\dot{E}_r, \dot{E}_D	energy rates due to reaction, diffusion respectively (equations 27, 28)
h	enthalpy
H	total enthalpy H
$I. N. I.$	incipient non-equilibrium index E/h (equation 12)
n	number of independent species in mixture
m	number of independent conservation laws relating species
M	equation (23)
p	pressure
\dot{p}_C	equation (9)
Pr	Prandtl number
q_i	species diffusional flux velocity
R	far wake radius
Re	Reynolds number

Sc	Schmidt number
t_c, t_f	chemical and fluid mechanic reference times respectively
T	temperature
\dot{t}_D, \dot{t}_{CD}	equation (9)
u, v	axial, radial velocities in wake
u_D	velocity defect in far wake (equation 15)
w_i	species mass generation rates due to chemical reactions
x, y	axial, radial coordinates in wake
δ	radius of near wake
Δ	equation (23)
\mathcal{E}	expansion parameter (equation 2)
Θ, Θ_h	equation (23)
μ	viscosity
ρ	density
Φ	equation (23)

Subscripts

0	condition at base corner in inviscid flow
1, 2	first, second terms in \mathcal{E} expansion
∞	free stream
b	base, or base surface
e	external (inviscid) flow
eq	in chemical equilibrium
Fr	frozen
i, j	i^{th}, j^{th} species
ref	high enthalpy reference condition (equation 26)

TABLE I

SUMMARY OF WAKE EXAMPLES

Far Wake (Turbulent Flow)

Case	Altitude kilofeet	Flight Speed ft/sec	Pressure atm.	Free Stream Stagnation temperature, °K
1	200	21,400	0.0002228	4630
2	150	21,400	0.001445	4885
3	100	21,000	0.0109	5380
4	70	21,000	0.04426	5710
5	70	18,000	0.04426	5320
6	70	15,000	0.04426	4680

Near Wake (Laminar Flow, 10° Sphere Cone, Flight Speed 21,400 ft/sec, $X_{\text{neck}}/R_b = 1.5$, $X/R_b = 1.7$)

Case	Altitude kilofeet	p/p_∞	Wall Temp. ratio, T_b/T_o	Wall Temperature T_b °K
7	150	3	0.5	2100
8	150	3	2.0	8400
9	50	2	0.5	1662.5
10	50	2	2.0	6650

VELOCITY ALONG CENTER LINE OF FAR WAKE

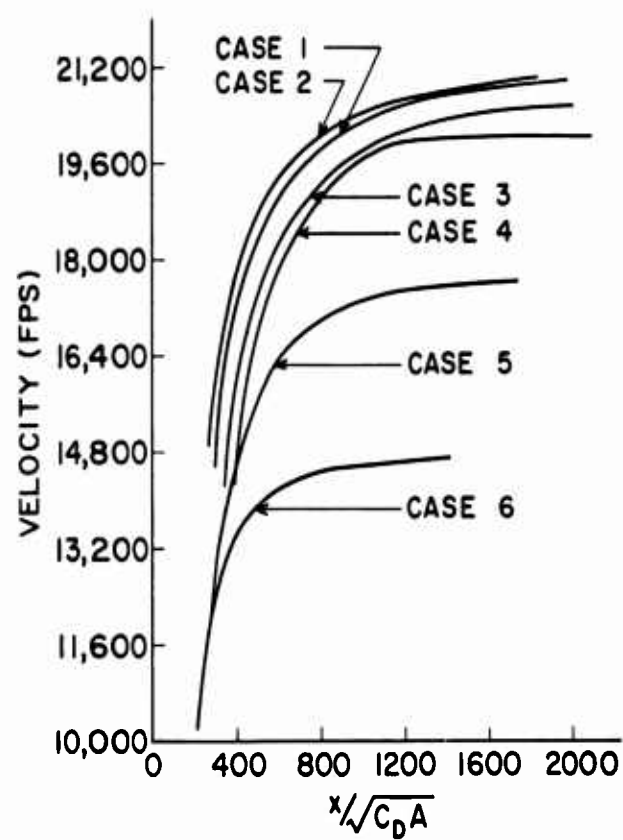


FIG. 1

TEMPERATURE ALONG CENTER LINE OF
FAR WAKE

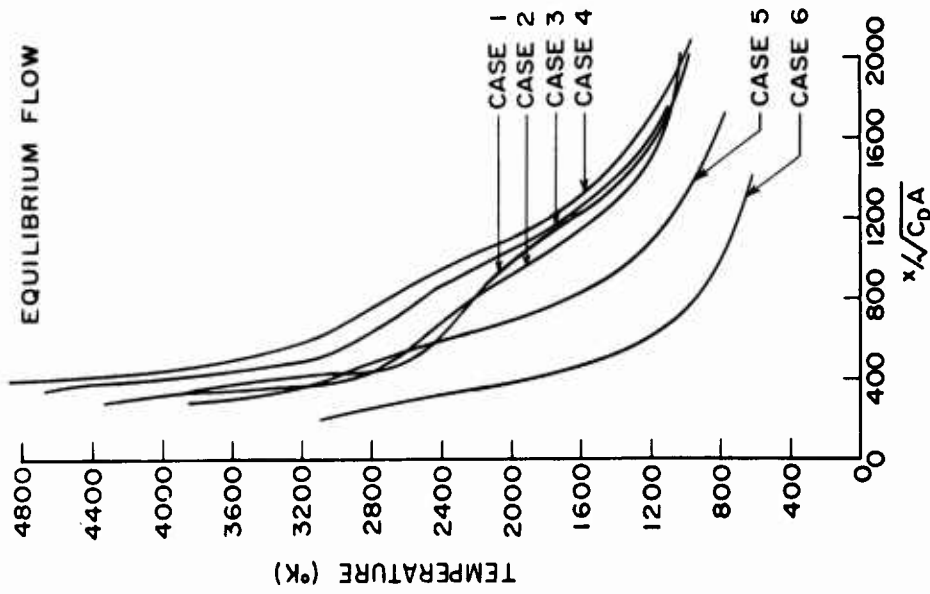


FIG. 2

ENTHALPY AND CHEMICAL ENERGY
ALONG CENTER LINE IN FAR WAKE

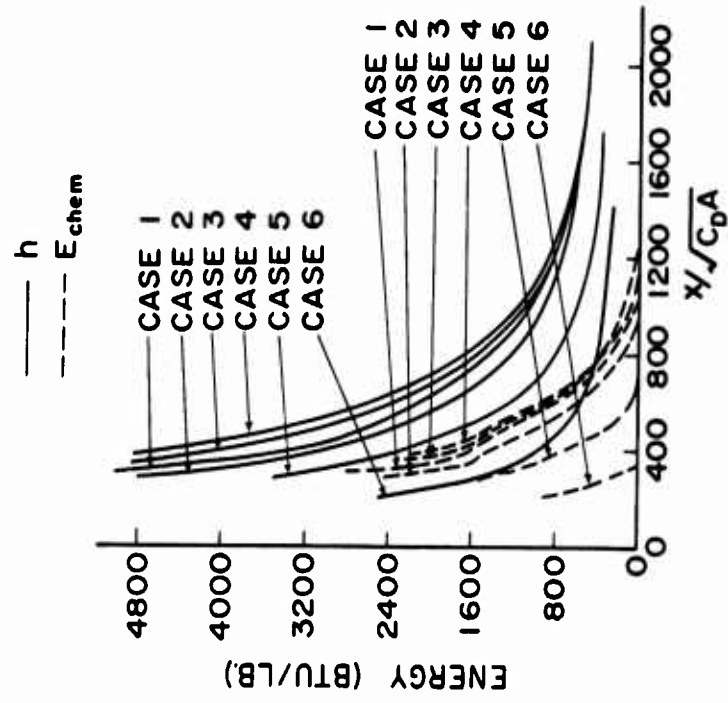


FIG. 3

INCIPIENT NON-EQUILIBRIUM INDEX ALONG WAKE CENTERLINE

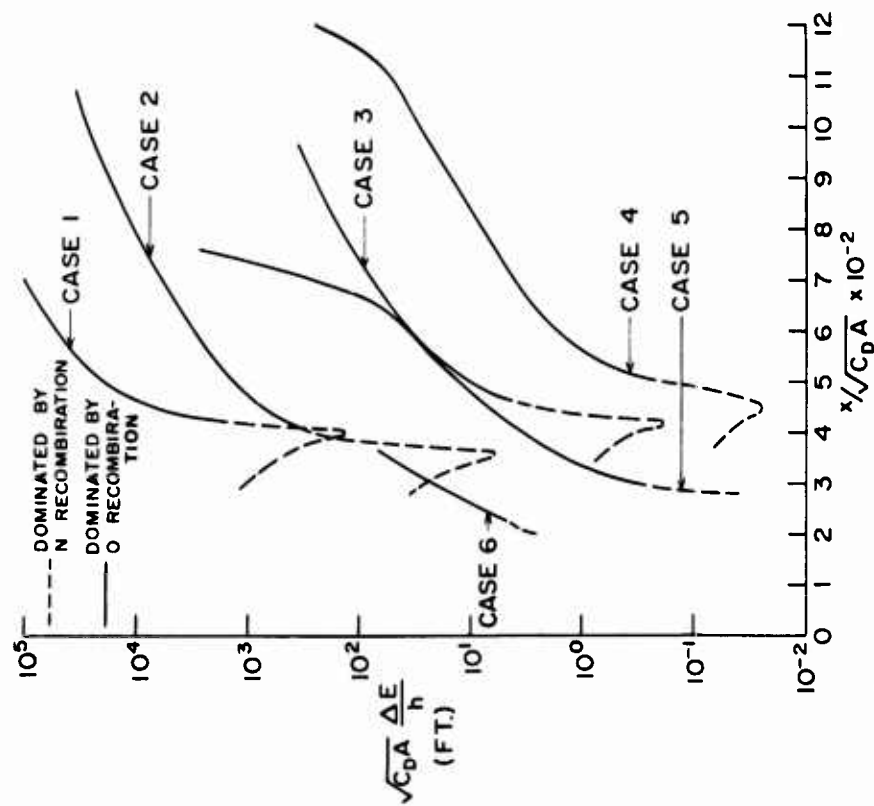


FIG. 4

VELOCITY AND TEMPERATURE PROFILE IN FAR WAKE

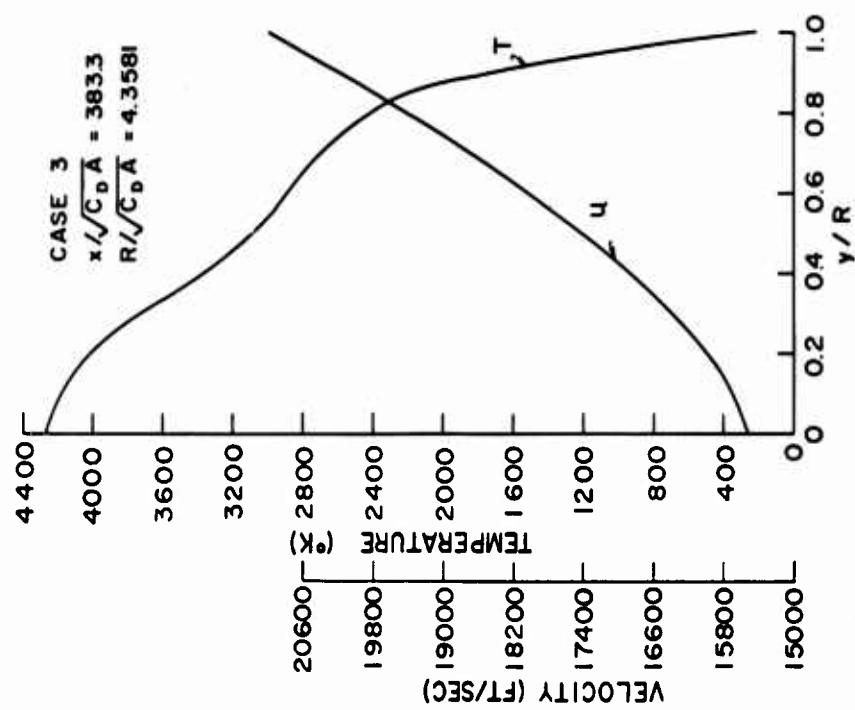


FIG. 5

ENTHALPY AND CHEMICAL ENERGY PROFILES IN FAR WAKE

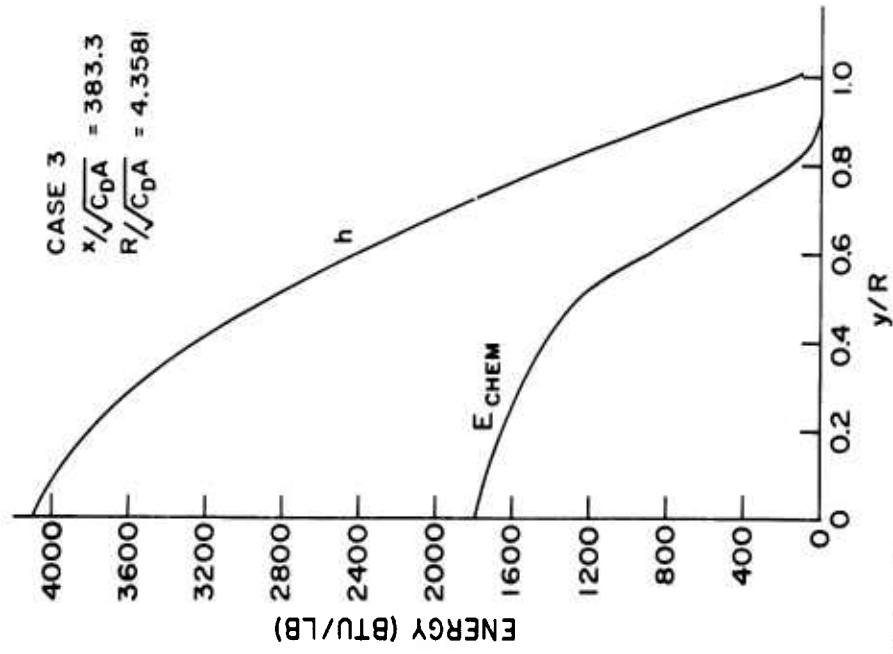


FIG. 6

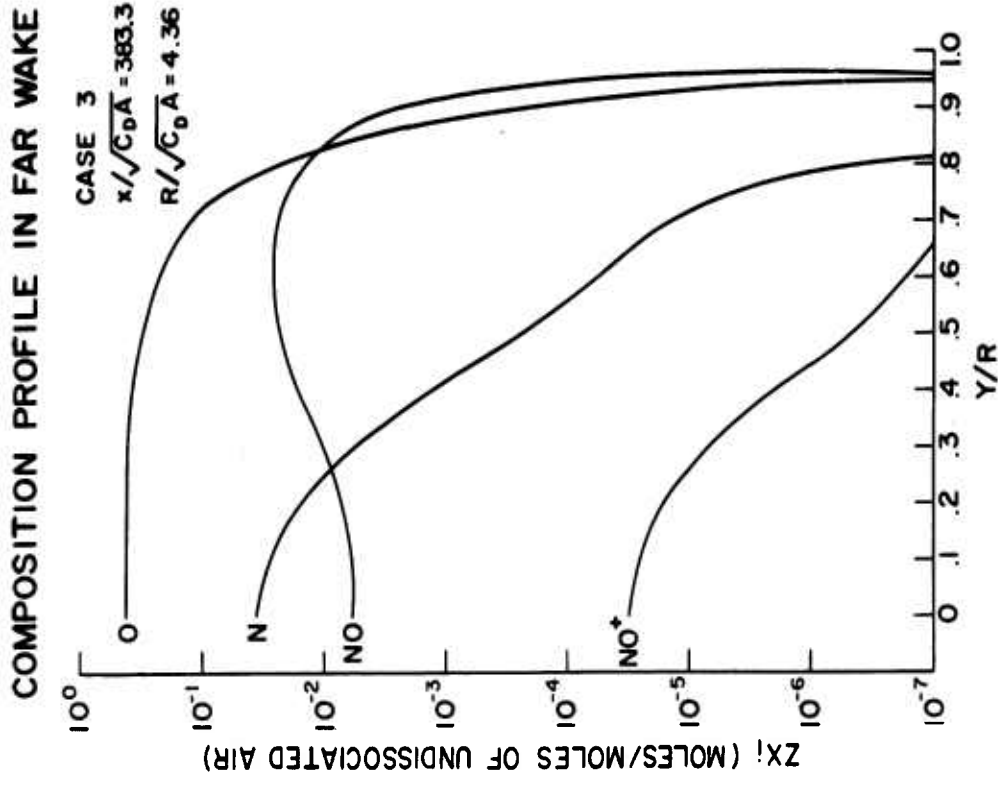


FIG. 7

INCIPIENT NON-EQUILIBRIUM INDEX IN FAR WAKE

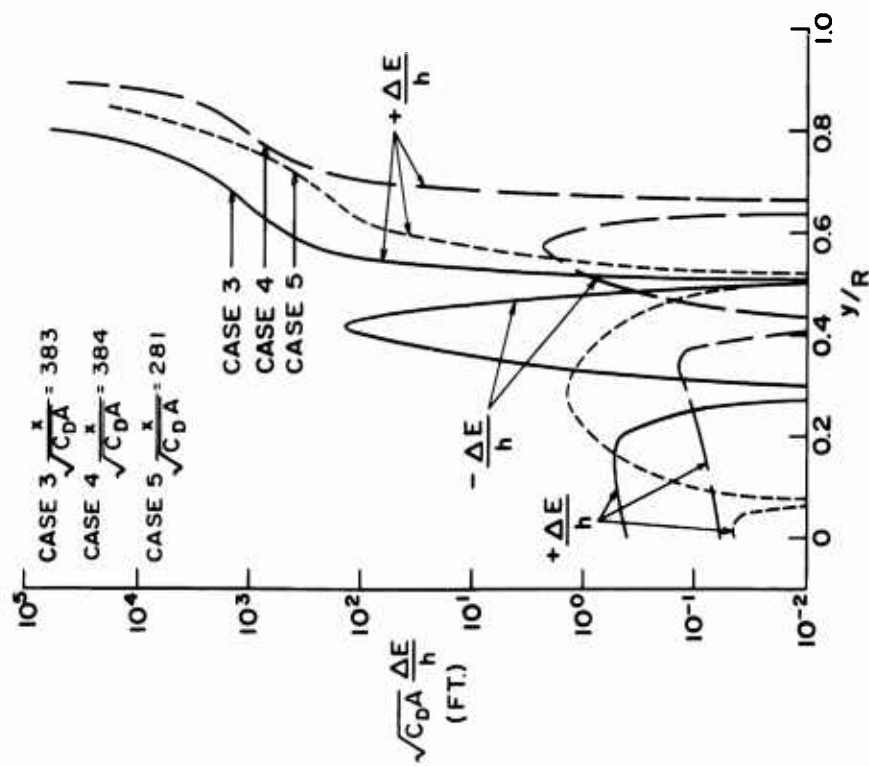


FIG. 8

INCIPIENT NON-EQUILIBRIUM INDEX IN FAR WAKE

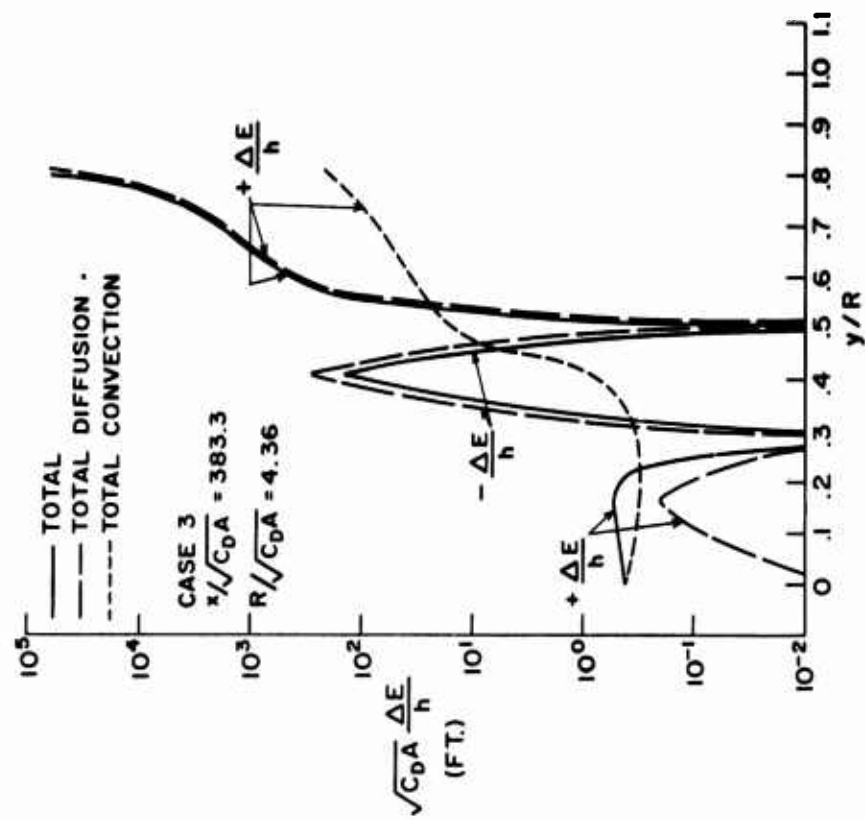


FIG. 9

INCIPIENT NON-EQUILIBRIUM INDEX
IN FAR WAKE
(DIFFUSION ONLY)

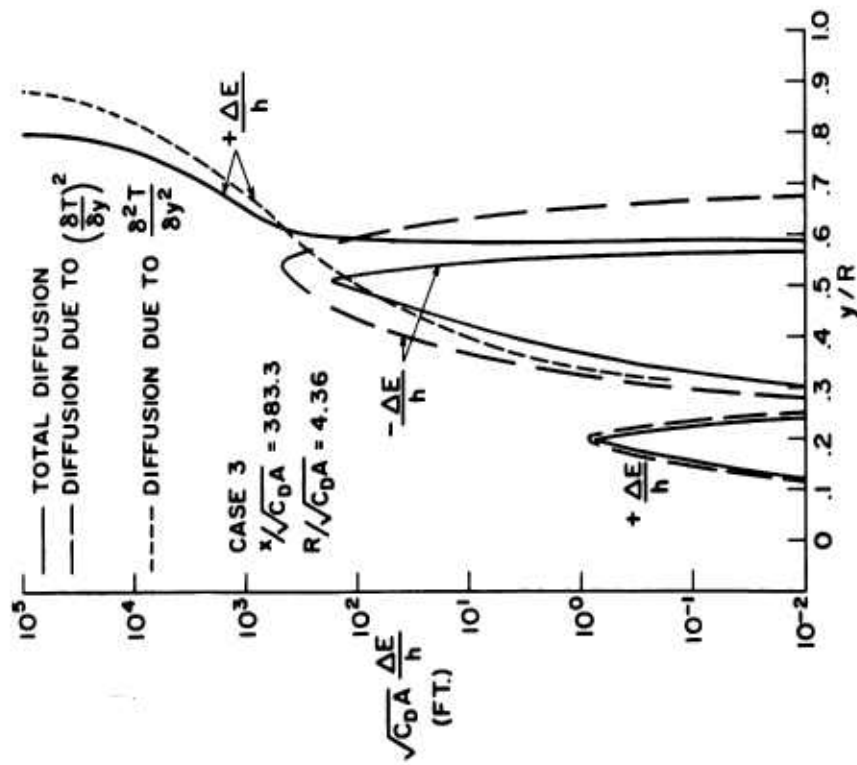


FIG. 10

INCIPIENT NON-EQUILIBRIUM INDEX IN FAR WAKE
(CONVECTION ONLY)

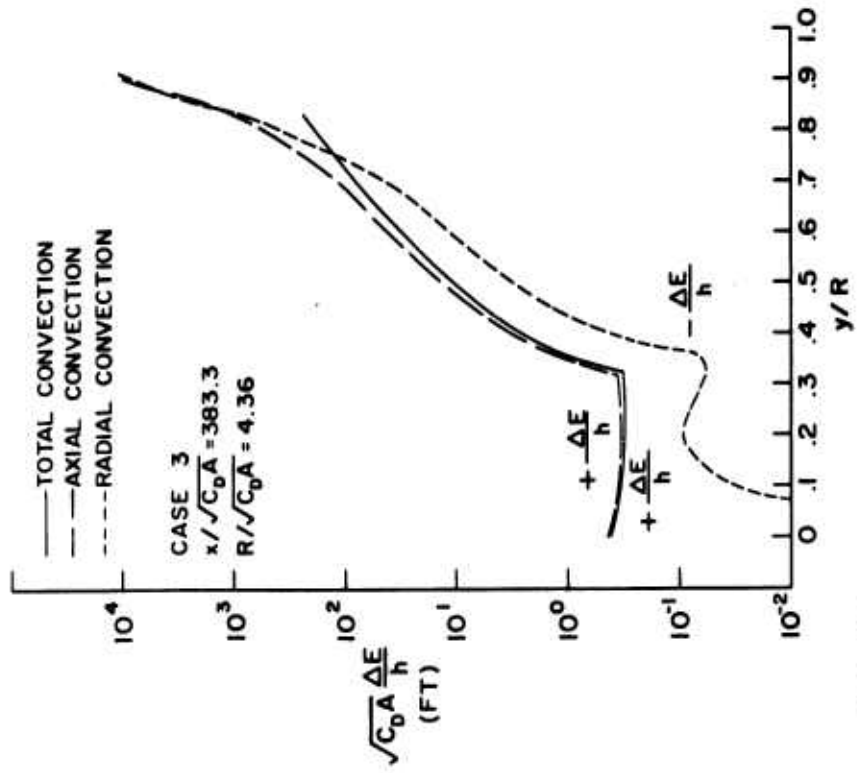


FIG. 11

INCIPIENT NON-EQUILIBRIUM INDEX IN FAR WAKE (EFFECT OF SPECIES)

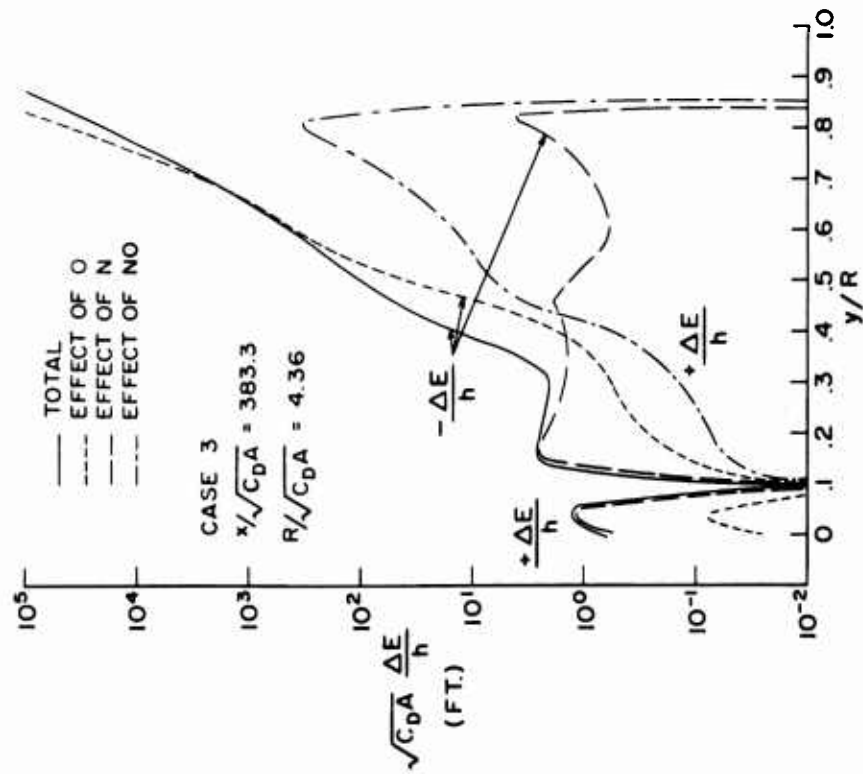


FIG. 12

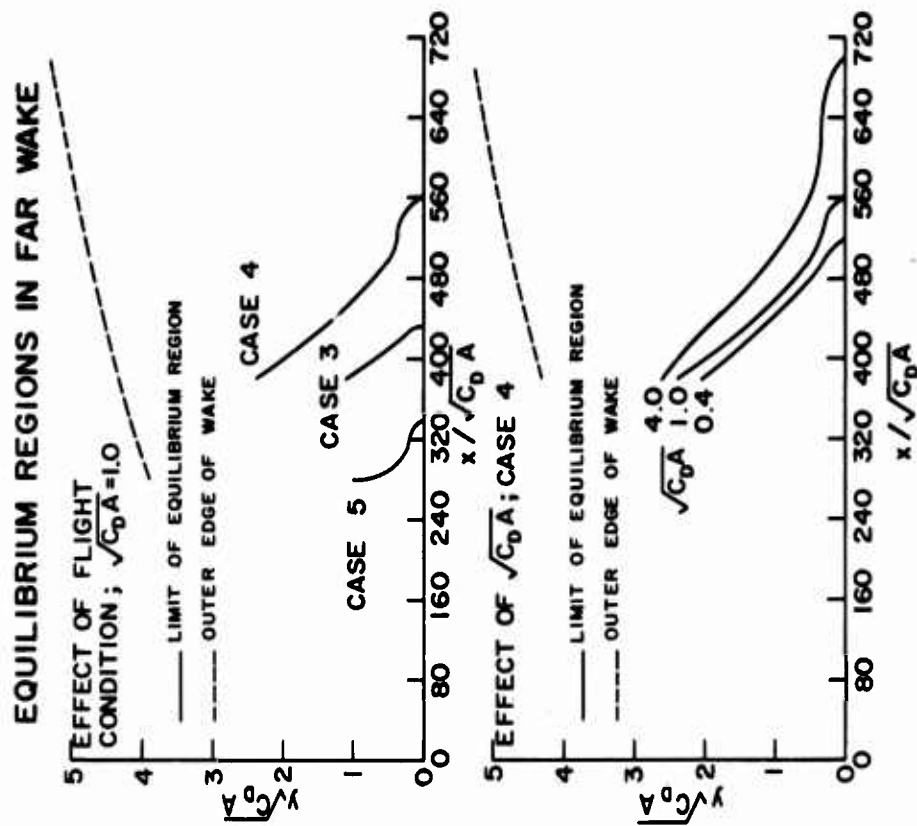


FIG. 13

EQUILIBRIUM TEMPERATURE PROFILES IN NEAR WAKE

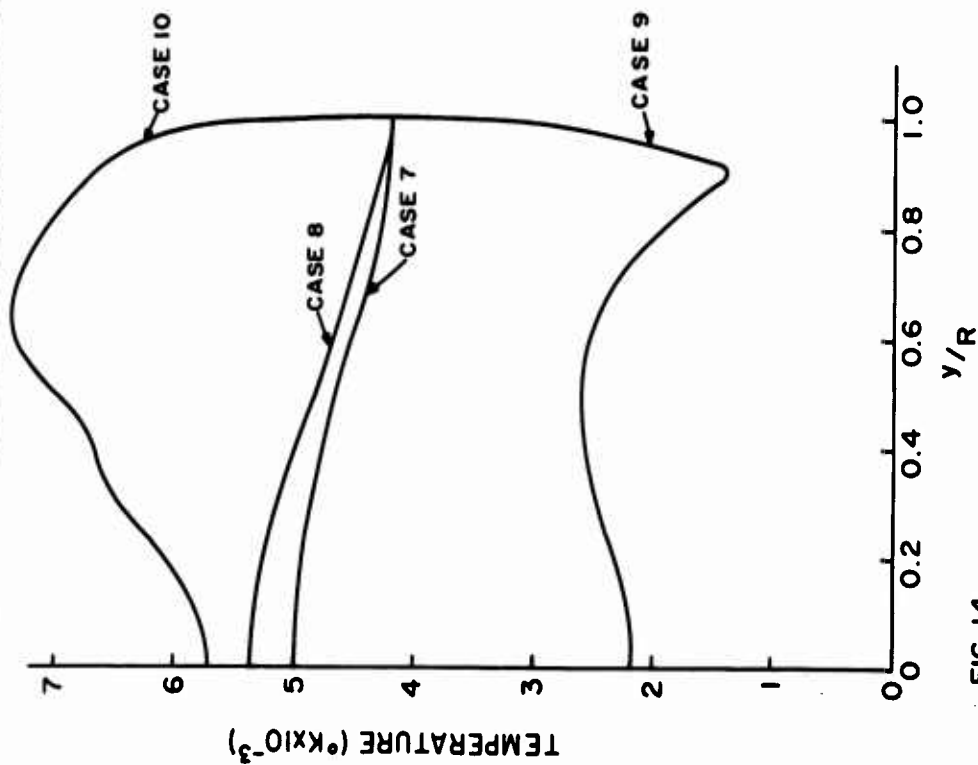


FIG.14

ENTHALPY AND CHEMICAL ENERGY IN THE NEAR WAKE

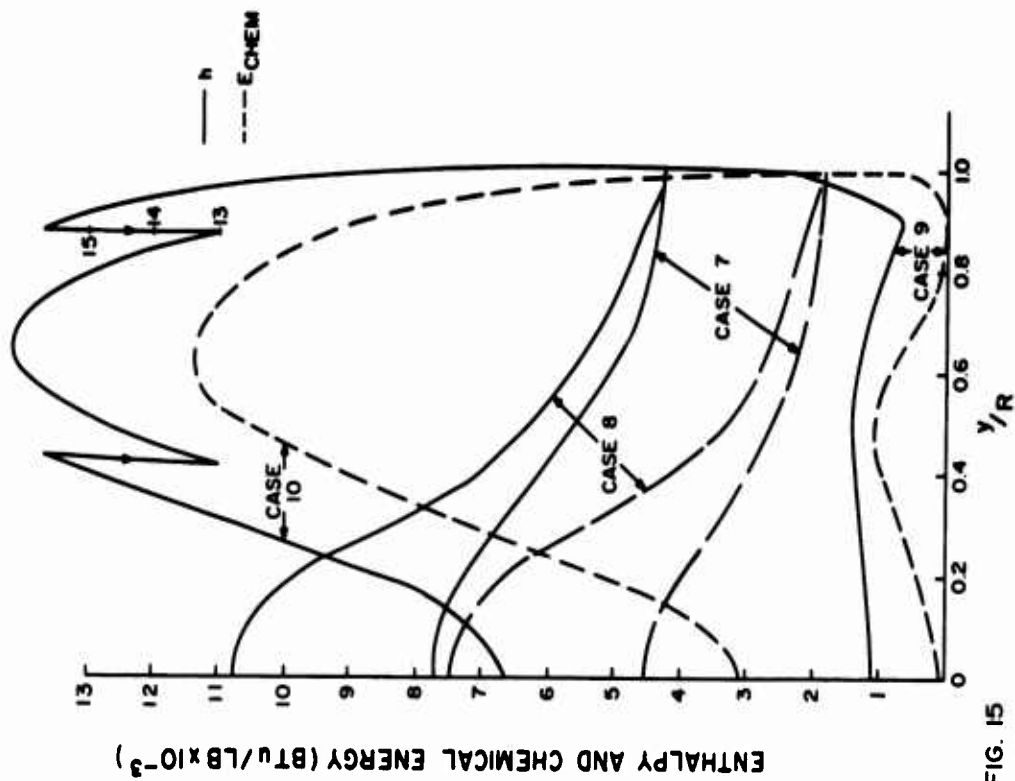


FIG.15

INCIPIENT NON-EQUILIBRIUM INDEX IN NEAR WAKE

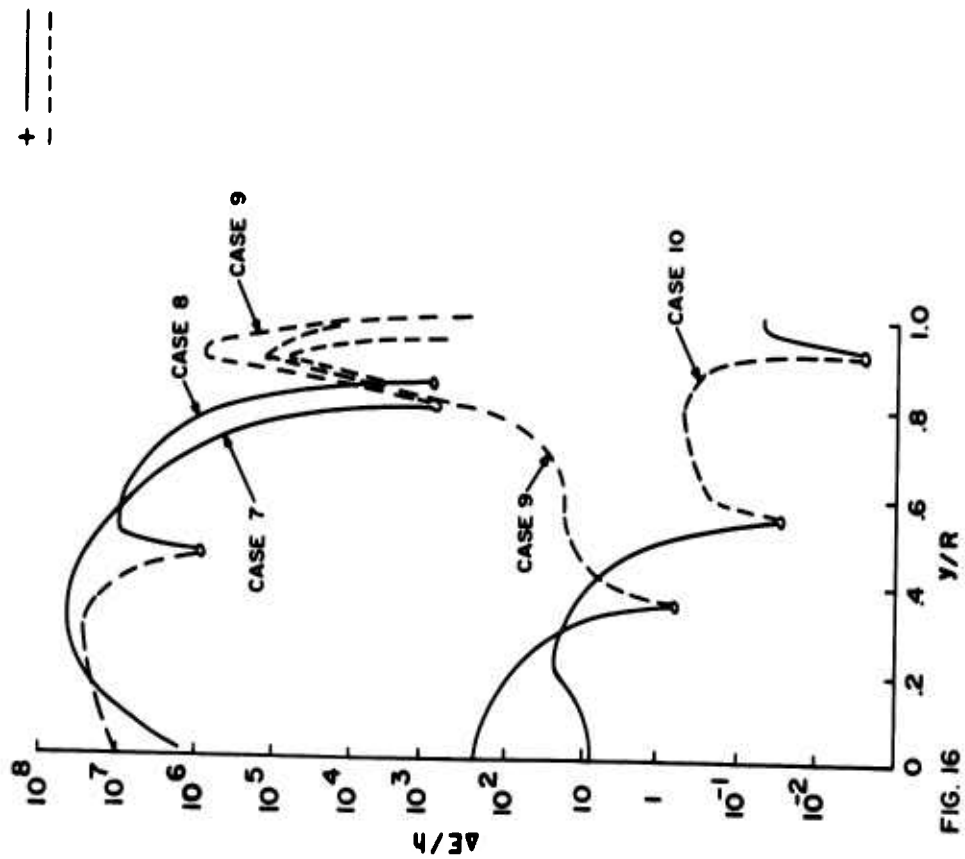


FIG. 16

INCIPIENT NON-EQUILIBRIUM INDEX IN NEAR WAKE

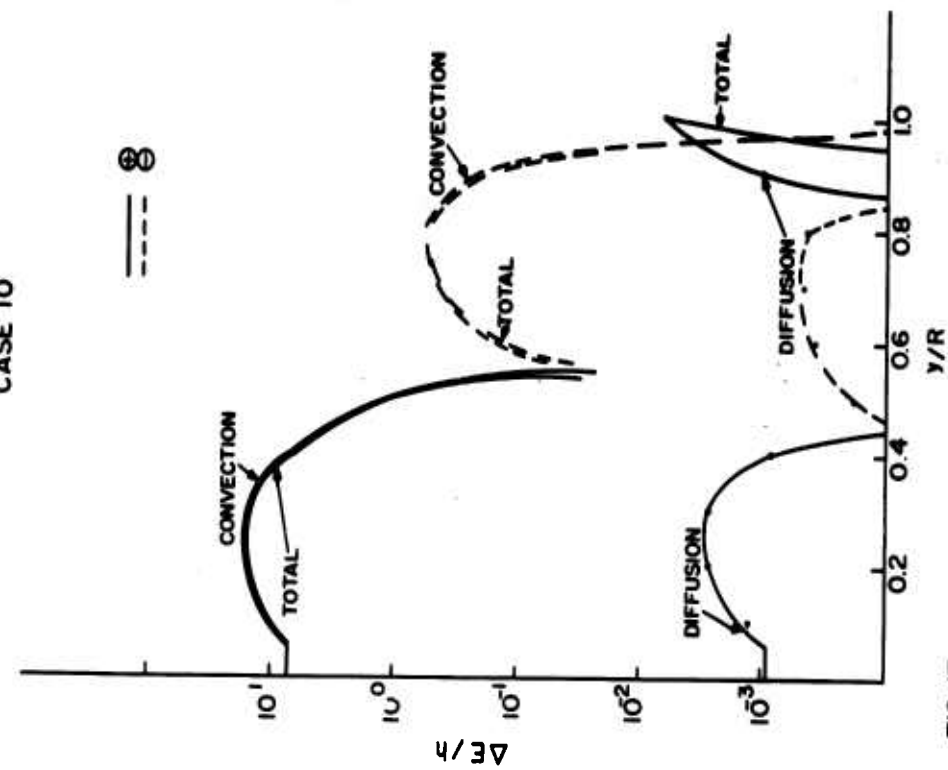


FIG. 17

FROZEN TEMPERATURE ALONG CENTER LINE OF FAR WAKE

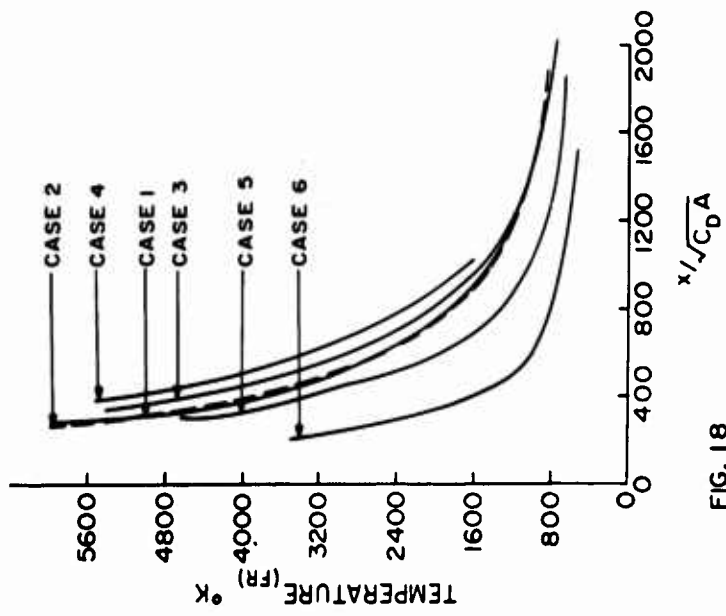


FIG. 18

VALIDITY OF CHEMICALLY FROZEN FLOW ALONG FAR WAKE CENTER LINE (T_{EQ})

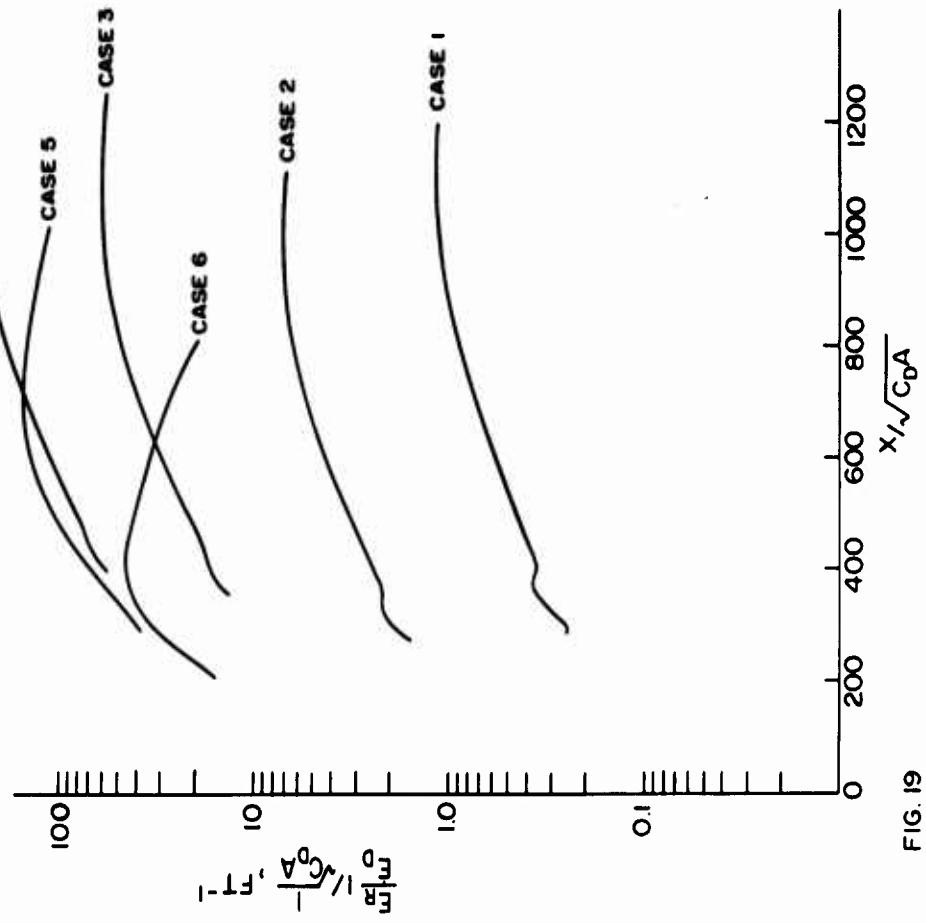


FIG. 19

VALIDITY OF CHEMICALLY FROZEN FLOW
ALONG FAR WAKE CENTER LINE (T_{FR})

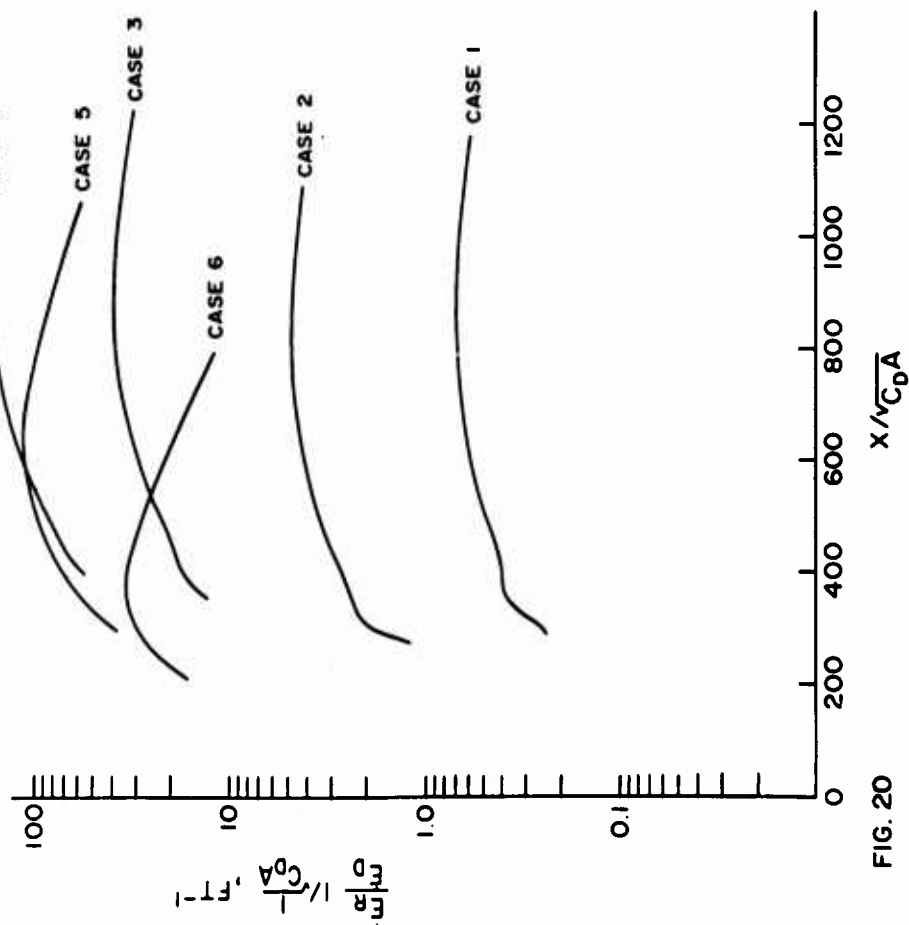


FIG. 20

FROZEN TEMPERATURE PROFILE IN FAR WAKE

CASE 3
 $X / \sqrt{C_0 A} = 383.3$
 $R / \sqrt{C_0 A} = 4.36$

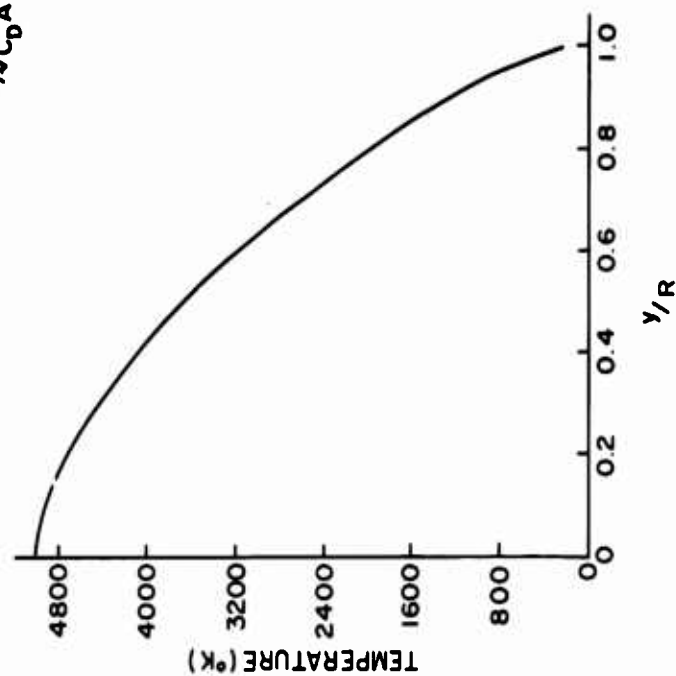


FIG. 21

VALIDITY OF CHEMICALLY FROZEN SOLUTION IN FAR WAKE PROFILE

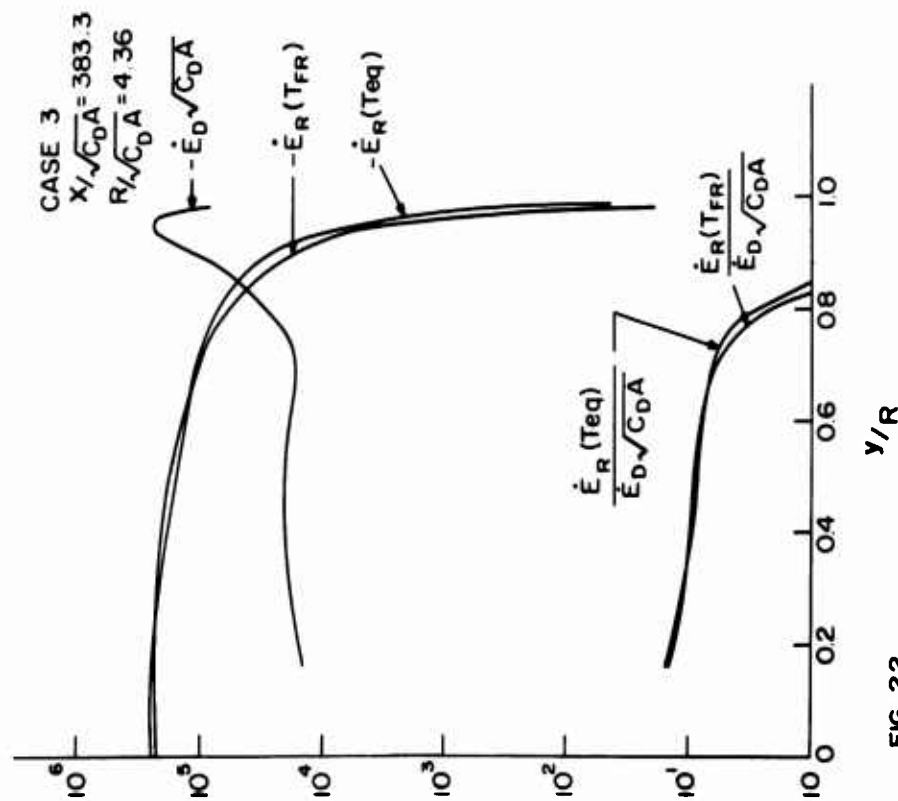


FIG. 22

ENERGY GENERATION RATES DUE TO SPECIES IN CHEMICALLY FROZEN FAR WAKE PROFILES (TEQ)

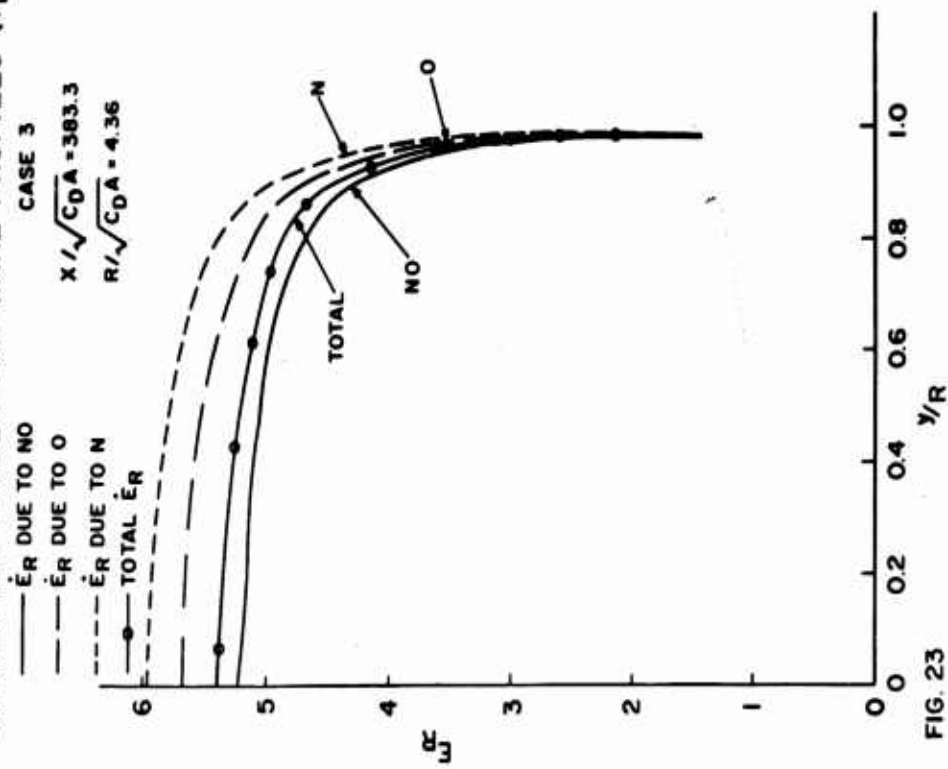


FIG. 23

ENERGY GENERATION RATES DUE TO SPECIES IN
CHEMICALLY FROZEN FAR WAKE PROFILE (T_{F_r})

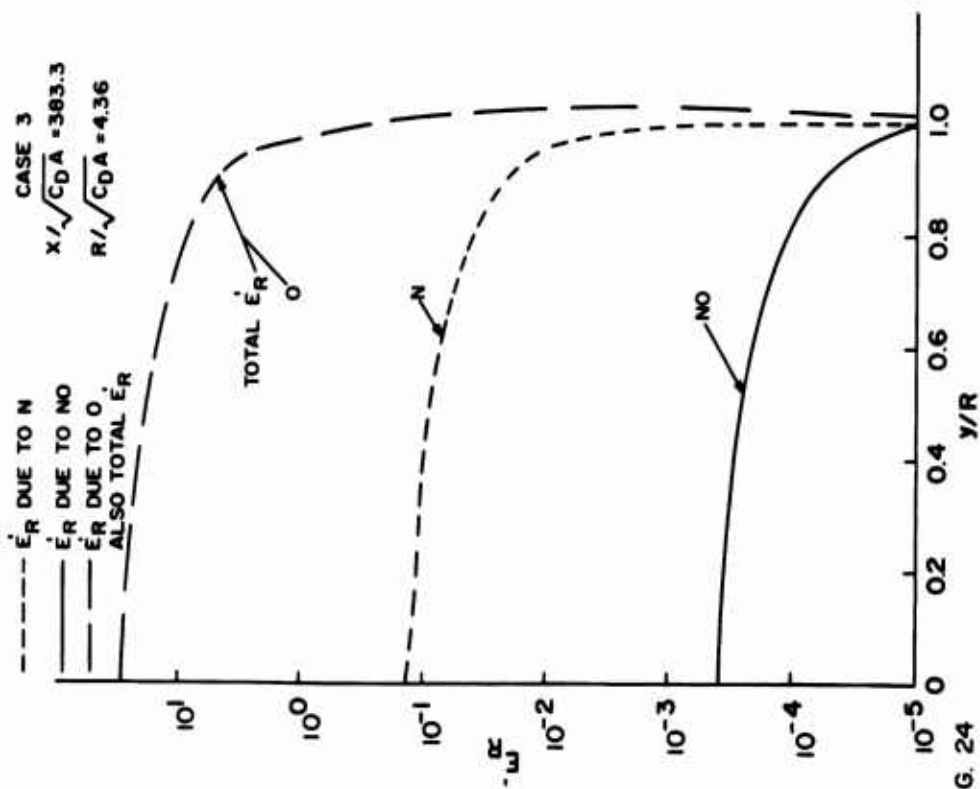


FIG. 24

FROZEN TEMPERATURE PROFILES IN NEAR WAKE

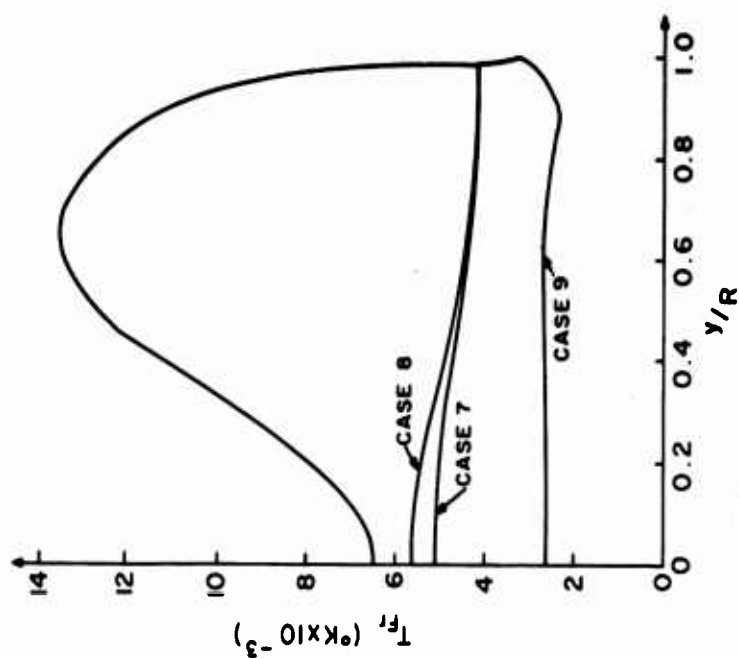


FIG. 25

VALIDITY OF CHEMICALLY FROZEN SOLUTION IN
NEAR WAKE PROFILE (T_{eq})

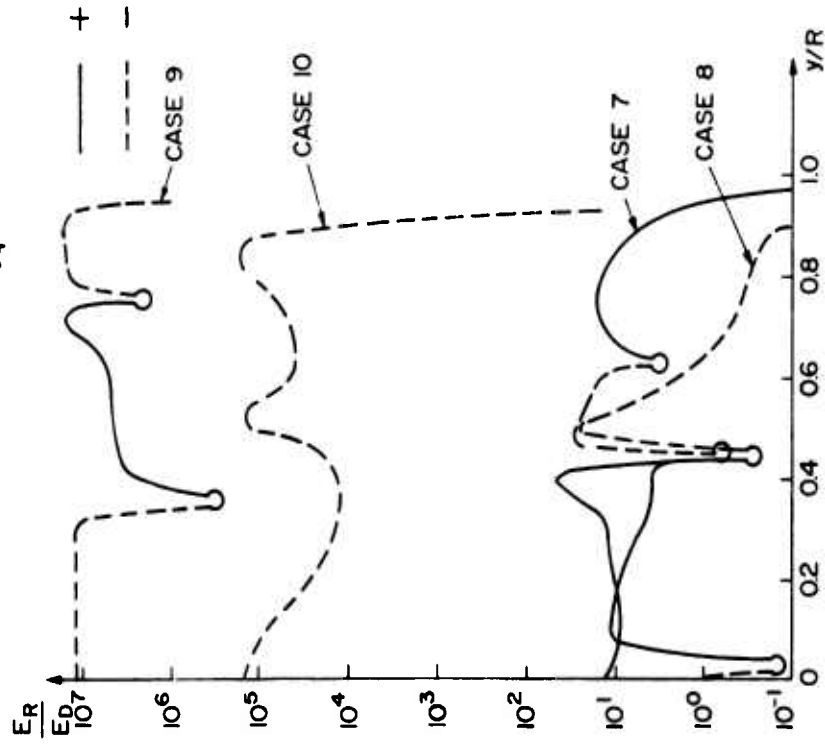


FIG. 26

VALIDITY OF CHEMICALLY FROZEN SOLUTION IN
NEAR WAKE PROFILE (T_{fr})

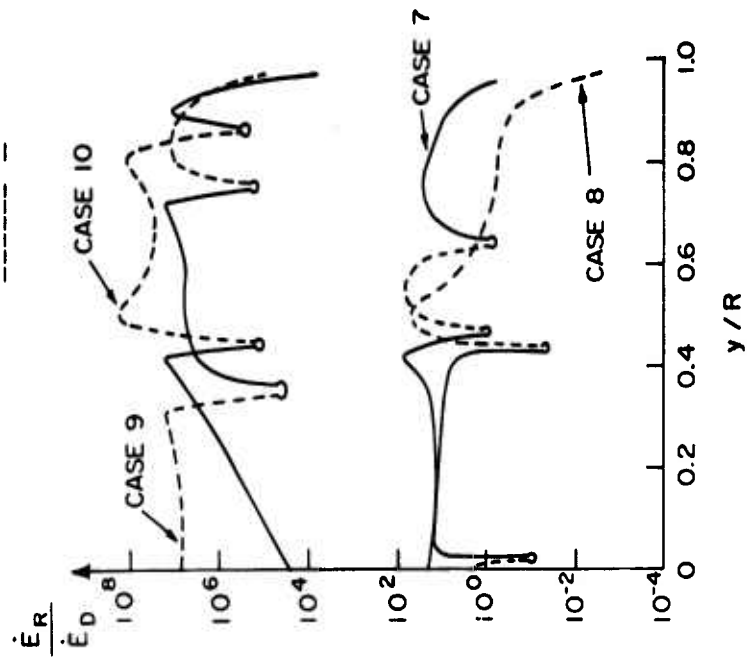


FIG. 27

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TECHNICAL INFORMATION SERIES

AUTHOR M. Lenard M. Long K. S. Wan	SUBJECT CLASSIFICATION Re-entry Physics	NO. R62SD989
		DATE Dec. 1962
TITLE CHEMICAL NON-EQUILIBRIUM EFFECTS IN HYPERSONIC PURE AIR WAKES		G. E. CLASS I
		GOV. CLASS None
REPRODUCIBLE COPY FILED AT MSD LIBRARY, DOCUMENTS LIBRARY UNIT, VALLEY FORGE SPACE TECHNOLOGY CENTER, KING OF PRUSSIA, PA.		NO. PAGES 36
SUMMARY The effect of finite chemical reaction rates on the chemical structure of hypersonic wakes is examined. The technique of incipient non-equilibrium coefficients, based on linearized chemical kinetics for a seven component (O_2 , N_2 , O , N , NO , NO^+ , e^-) ten reaction model of high temperature air, is utilized in the analysis. The far wake is treated as an asymptotic region; the near wake theory considers the viscous mixing of the boundary layer flow with the inviscid and re-circulating flows in the base region, and the subsequent development of this viscous core into the wake region downstream. The results show where non-equilibrium effects are important in the wake and why they arise. The incipient non-equilibrium results are then related to calculations assuming chemically frozen flow.		

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AUTHOR Michael Lenard, M. Long, K. S. Wan
COUNTERSIGNED A. G. Lewis, Joseph F. Fisher

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